

Temperature dependent band structure of the Kondo insulator

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We present a Quantum Monte Carlo (QMC) study of the temperature dependent dynamics of the Kondo insulator. Working at the so-called symmetrical point allows to perform minus-sign free QMC simulations and thus reach temperatures of less than 1% of the conduction electron bandwidth. Study of the temperature dependence of the single particle Green's function and dynamical spin correlation function shows a surprisingly intricate low temperature band structure and gives evidence for two characteristic temperatures, which we identify with the Kondo and coherence temperature, respectively. In particular, the data show a temperature induced metal-insulator transition at the coherence temperature.

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The theoretical description of the Kondo lattice remains an outstanding problem of solid state physics. This model, or variations of it, may be viewed as the appropriate one for understanding such intensively investigated classes of materials as the heavy electron metals [1,2] and the Kondo insulators [3]. Experimental results indicate that the electronic structures of Kondo lattice compounds undergo quite dramatic changes with temperature [4]. It is the purpose of the present manuscript to report a QMC study of the electronic structure of the so-called Kondo insulator, which shows that this model indeed undergoes a quite profound change of its unexpectedly intricate band structure as temperature increases. We are using a one dimensional (1D) 'tight-binding version' of the model with L unit cells and 2 orbitals/unit cell:

$$H = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + H.c.) - V \sum_{i,\sigma} (c_{i,\sigma}^\dagger f_{i,\sigma} + H.c.) - \epsilon_f \sum_{i,\sigma} n_{i,\sigma} + U \sum_i f_{i,\uparrow}^\dagger f_{i,\uparrow} f_{i,\downarrow}^\dagger f_{i,\downarrow}. \quad (1)$$

Here $c_{i,\sigma}^\dagger$ ($f_{i,\sigma}^\dagger$) creates a conduction electron (f -electron) in cell i , $n_{i,\sigma} = f_{i,\sigma}^\dagger f_{i,\sigma}$. Throughout we consider the case of 'half-filling' i.e. two electrons/unit cell and, as an important technical point, we restrict ourselves to the symmetric case, $\epsilon_f = U/2$. The latter choice, while probably not leading to any qualitative change as compared to other ratios of ϵ_f/U , has the crucial advantage that at half-filling the model acquires particle-hole symmetry, i.e. the Hamiltonian becomes invariant under the transformation $\alpha_{i,\sigma} \rightarrow \exp(i\mathbf{Q} \cdot \mathbf{R}_i) \alpha_{i,\sigma}^\dagger$, where $\alpha = c, f$ and $\mathbf{Q} = (\pi, \pi, \dots)$ (this holds for bipartite lattices with only nearest neighbor hopping). Particle-hole symmetry in turn implies that the QMC-procedure does not suffer from the notorious 'minus-sign problem' anymore, so that reliable simulations for temperatures as low as $\beta t = 30$, corresponding to $\approx 0.8\%$ of the conduction electron bandwidth, can be performed without problems. This allows to scan the dynamical correlation functions

of the system over a wide temperature range. Previously a QMC study for the 2 dimensional model at half-filling was performed by Vekic *et al.* [5], more recently a study of the temperature dependence of *static* susceptibilities for the strong coupling version of the model has been reported by Shibata *et al.* [6].

It is widely believed that the Kondo lattice has two distinct characteristic temperatures. At the Kondo temperature, T_K , the f -electrons start to form loosely bound singlets with the conduction electrons. This manifests itself in a deviation of the spin susceptibility from the high-temperature Curie form due to the 'quenching' of the f -electron magnetic moment and an increase of the dc-resistivity due to resonant scattering from the newly formed low energy bound states [1]. The second (and lower) characteristic temperature is the coherence temperature, T_{coh} , where the local singlets establish long range coherence amongst themselves so as to participate in the quasiparticle bands of a Fermi-liquid like electronic state. Experimentally the coherence temperature is signaled by the onset of a decrease of the dc resistivity with temperature [1], and the formation of the 'heavy bands' which (judging by the volume of the Fermi surface) incorporate the f -electrons [7]. While there is as yet no experimental proof, one might expect on the basis of these considerations, that at temperatures above T_{coh} the f -electrons do not participate in the Fermi surface volume, whereas they do so below.

Turning to the Kondo insulator we note that the electron count for these systems is such that the 'Fermi surface' comprising both, conduction and f -electrons, would precisely fill the Brillouin zone so that the system is a 'nominal' band insulator. If increasing temperature causes the f -electrons to 'drop out' of the Fermi surface volume, this should manifest itself as an insulator-to-metal transition because the volume of the collapsed Fermi surface is no longer sufficient to cover the entire Brillouin zone. Transferring the above scenario for heavy Fermion metals to the Kondo insulator one would therefore expect that the

system remains a metal above T_{coh} , with a Fermi surface that excludes the f -electrons, and becomes insulating below T_{coh} , when the f -electrons participate in the Fermi surface volume to turn the system into a ‘nominal’ band insulator. In fact insulator-to-metal transitions which are induced by temperature [4], or hydrostatic pressure [8] have been observed experimentally. As will be seen below, our data for the Kondo insulator are remarkably consistent with such an interpretation.

To begin with, we consider the T -dependence of the single particle spectral function. This is defined as ($\alpha=c, f$)

$$A_\alpha(k, \omega) = \frac{1}{Z} \sum_{\nu, \mu} e^{\beta \omega_{\nu\mu}} |\langle \nu | \alpha_{k, \sigma} | \mu \rangle|^2 \delta(\omega - \omega_{\nu\mu}), \quad (2)$$

where the sum is over all eigenstates $|\nu\rangle$ of $H - \mu N$ in the grand canonical ensemble, Z denotes the partition function and $\omega_{\nu\mu}$ the difference of the energies of the states ν and μ . Figure 1 shows the angle-integrated spectral

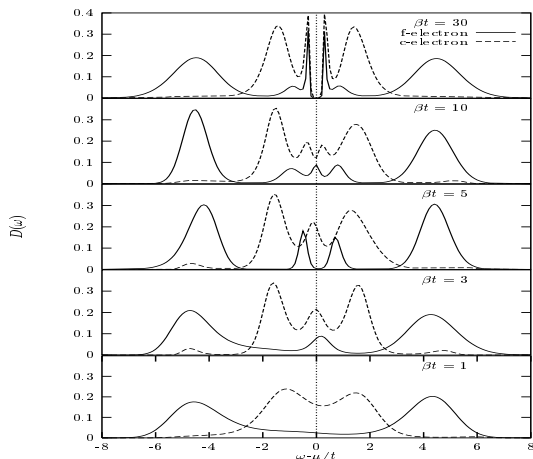


FIG. 1. Angle integrated spectral density $D(\omega)$ for an $L=16$ Kondo lattice for different temperatures. Parameter values are $U/t=8$, $V/t=1$.

density, $D_\alpha(\omega) = (1/L) \sum_k A_\alpha(k, \omega)$. At the lowest temperature, $\beta t=30$, $D_\alpha(\omega)$ shows the behaviour expected for a Kondo insulator: the c -electron density is roughly consistent with the standard 1D tight-binding density of states, with indications of the two van-Hove singularities at $\pm 2t$. Around μ , however, the spectral density shows a small but unambiguous gap, which demonstrates the insulating nature of the ground state. The f -like spectral density shows very sharp low energy peaks at the edges of this gap, as well as high-intensity ‘Hubbard bands’ at approximately $\pm U/2$. There are also two weak ‘side bands’ at approximately $\pm 0.8t$. With the exception of these, all features are consistent with exact diagonalization [9] and $d \rightarrow \infty$ results [10] at $T=0$. This suggests that the sidebands are already an effect of the finite temperature and the further development with T confirms this. Inspection of the series $\beta t=30, 10$ shows that with increasing T

a transfer of spectral weight from the low energy peaks at the gap-edges into the sidebands is taking place. This is accompanied by a narrowing of the gap, and at $\beta t=10$ the gap practically closes; in the spectrum for this temperature the two low-energy peaks seem to have collapsed into a single one right at μ - we believe that these are in fact still two peaks, which however are too closely spaced to be resolved. Increasing T even further ($\beta t=5$), the low energy peaks disappear completely. The c -electron spectral density no longer shows any indication of a gap, whereas the f -like sidebands stay at a relatively high energy away from μ . The extreme low energy states thus have pure c -character (within the resolution of the QMC procedure) and the system is a metal with a c -like Fermi surface. We therefore interpret the temperature where the gap closes as the analogue of the coherence temperature. With increasing T the energy of the sidebands is lowered and at $\beta t=3$ they collapse into a single peak right at μ . This probably indicates a second transition and at the relatively large value of $\beta t=1$ another reconstruction of the band structure has taken place, namely the disappearance of the f -like sidebands. The upper and lower Hubbard band for the f -electrons are now quite broad, and actually the possibility that there are very low-intensity f -like features near μ cannot be completely ruled out. However, the overall trend is quite obviously a strong decrease of the sidebands. Interpreting the latter as the lattice-analogue of the Kondo-resonance in the impurity case [11], the temperature of the second transition should correspond to the Kondo temperature T_K . In the present case T_K is very high because of the relatively large value of the c - f hybridization, $V=t$. We also note that the closing of a gap in the f -like density of states in 2 dimensions was previously found by Vekic *et al.* [5].

To get a more detailed picture, we consider the k -resolved single particle spectral function, shown in Figure 2 for some temperatures in between the two transitions. For $\beta t=30$ the c -electrons show a standard $\cos(k)$ band, albeit with a clear gap at $k_F^0 = \pi/2$, the Fermi momentum of nonhybridized conduction electrons. At this momentum the band changes its spectral character and ‘bends over’ into a practically dispersionless f -like band, which can be followed up to $k=\pi$. This kind of band structure is familiar from various studies [9,10,12]. The weak and practically dispersionless f -like sidebands are at somewhat higher energy and, at very high energies, the f -like Hubbard bands. The width of the Hubbard bands seems to depend strongly on momentum - this is a deficiency of the QMC and maximum entropy method, which is most accurate near μ . As seen in the k -integrated spectra, raising the temperature leads to a transfer of spectral weight from the ‘flat band’ forming the single-particle gap into the Kondo resonance-like sidebands. At $\beta t=5$, where the gap has closed, the c -electron spectrum shows a very conventional $\cos(k)$ -band with no more indication of any gap. At k_F^0 there is now one symmetric and un-

split peak right at μ - as it is required by particle-hole symmetry for a metallic system. The system thus has a

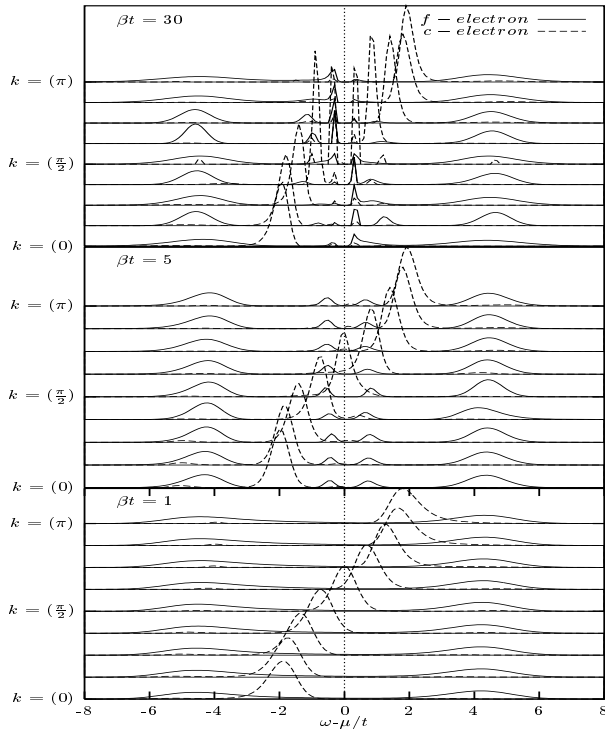


FIG. 2. Momentum resolved single-particle spectral function $A(k, \omega)$ at different temperatures. Parameters as in Figure 1, the momentum k increases in steps of $2\pi/L = \pi/8$ from the bottom of each panel.

Fermi surface as expected for unhybridized c -electrons, i.e. the f -electrons indeed have ‘dropped out’ of the Fermi surface volume. The dispersionless f -like sidebands are at a relatively high energy. The tiny low energy ‘foot’ seen in some of the c -like spectra may indicate a very weak mixing of the c -electrons into the Kondo-resonance but apparently this no longer leads to a gap. Rather, the Kondo resonance is now essentially decoupled from the Fermi surface physics. Finally, for $\beta t = 1$, even these Kondo resonance-like sidebands have disappeared and the only f -like peaks in the spectral function are the upper and lower Hubbard bands. At this high temperature the f -electrons do not participate in the low energy physics at all. The expectation value of $-V \sum_{i,\sigma} (c_{i,\sigma}^\dagger f_{i,\sigma} + H.c.)$ decreases by $\approx 30\%$ between $\beta t = 30$ and $\beta t = 1$ - while there is appreciable mixing even at high temperature, this does obviously not lead to coherent band formation any more.

We proceed to the dynamical spin correlation function (SCF), defined as

$$S(k, \omega) = \frac{1}{Z} \sum_{\nu, \mu} e^{-\beta E_\mu} |\langle \nu | S_\alpha^z(k) | \mu \rangle|^2 \delta(\omega - \omega_{\nu\mu}), \quad (3)$$

where $S_\alpha^z(k)$ is (the Fourier transform of) the z -

component of the spin-operator for α -electrons. This is shown in Figure 3. At $\beta t = 30$, the f -like SCF shows an intense branch of low energy excitations with a tiny but clearly resolved spin wave-like dispersion. The spectral weight of this branch is sharply peaked at $k = \pi$, indicating relatively long ranged and strong antiferromagnetic spin correlations. Fitting the equal (imaginary) time f -like spin correlation function in real space to the expression $S(r) = A(e^{-r/\zeta} + e^{-(L-r)/\zeta})$ we obtain the values $\zeta = 4.61, 4.67$ and 2.18 for $\beta t = 30, 20$ and 10 . The dominant feature in the c -like SCF on the other hand, is a free electron-like particle-hole continuum. Interestingly enough, there is also a replica of the f -electron spin wave branch in the c -like SCF. This shows that at low excitation energies c and f electrons behave as a single ‘all-electron fluid’, whose excitations have composite f - c character. The free electron continuum itself does have a gap of $\approx 0.6t$ at $k = \pi$ - this corresponds to approximately

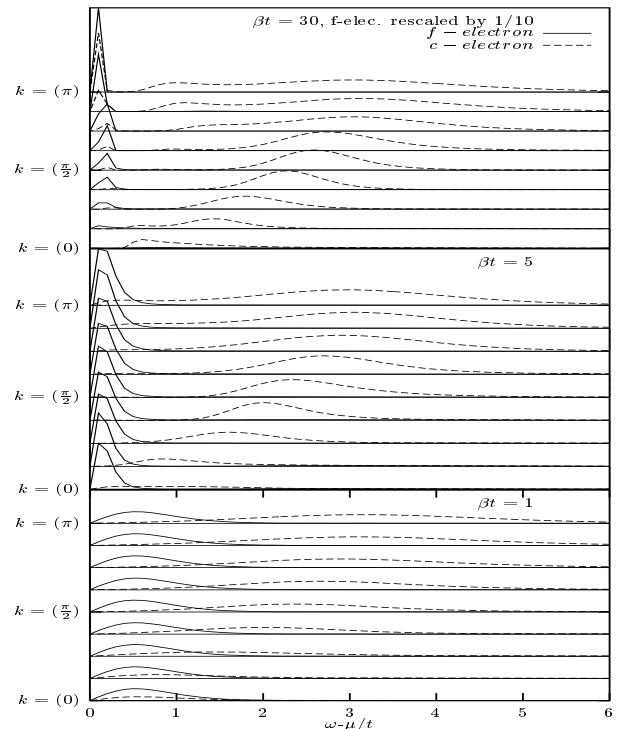


FIG. 3. Dynamical spin correlation function $S(k, \omega)$ for different temperatures. Parameters are as in Figure 1.

twice the single particle-gap in $A(k, \omega)$ [13]. We proceed to $\beta t = 5$, where the single-particle gap has closed. The f -like SCF still shows a low-energy peak with finite excitation energy, which however is practically dispersionless, both with respect to its energy and with respect to its spectral weight. In other words, the magnetic f -excitation becomes practically immobile. The metal-insulator transition thus is related to a drastic change of the spin correlation function [5] - the question whether the longer ranged spin correlations below the transition

are the driving force behind the gap formation [13] or whether the change of the spin correlations is merely a ‘byproduct’ of the collapse of the single-particle gap, remains to be clarified. In any way, the almost completely localized spin dynamics of the f -electrons naturally should lead to a Curie-law for the static spin susceptibility at temperatures above T_{coh} . A crossover from an activation-gap dominated susceptibility at low temperatures and a Curie law at high temperatures has indeed been observed by Shibata *et al.* [6]. In the c -like SCF the particle-hole continuum persists and the gap near $k=\pi$ is now very small or zero (the absence of the gap in the single particle spectrum suggests it to be zero). There is no more distinguishable peak in the c -like SCF which would correspond to the dispersionless f -like spin resonance - this suggests that the f -electrons now are largely decoupled from the c -like band, as indicated by their non-participation in the Fermi surface. At the very high $\beta t=1$, there is still some (very weak) indication of the low energy f -electron spin resonance, but the intensity is low and the resonance is now relatively broad. It should be noted that the relative change of the f -like magnetic moment is less than 2% over the entire temperature range we studied - temperature thus affects only the coupling of these moments to the conduction electrons.

For the relatively large value of $V=1$ the higher of the two crossover temperatures (i.e. the Kondo temperature) is already rather high, $\beta t \geq 1$. Based on the impurity results [14] one might expect that for smaller V the Kondo temperature is lower, and to check this, we have performed

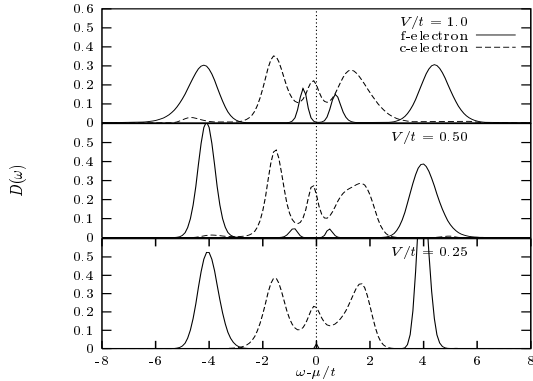


FIG. 4. Single particle spectral density $D(\omega)$ at $\beta t=5$ for different V/t . All other parameters are as in Figure 1.

simulations at fixed $\beta t=5$, but with variable hybridization. Figure 4 shows the results for the single particle spectral density. The weight of the Kondo resonance-like sidebands for fixed temperature decreases with V , and for $V/t=0.25$ they have disappeared completely. In the k -resolved c -electron spectrum (not shown) there is now only a very sharp nearest neighbor-hopping band with a clear Fermi level crossing at k_F^0 and the f -like

spin correlation function shows no more indication of the low energy resonance - the overall picture is completely the same as for $V/t=1$ and $\beta t=1$, with the sole exception that all features are much sharper due to the lower temperature. Here we do not pursue the issue of the detailed parameter dependence of the characteristic temperatures - it is quite obvious, however, that lower values of V shift the characteristic temperatures of the system towards lower values, but otherwise leave the physics unchanged.

In summary, we have studied the temperature evolution of various dynamical correlation functions of the Kondo insulator and found indications for two distinct electronic crossovers. At the low temperature crossover the single-particle gap closes so that the system becomes a metal, the magnetic correlations on the f -sites become localized, and the ‘spin gap’ closes due to c -like spin excitations. While c and f electrons seem to form a coherent ‘all-electron fluid’ below the crossover temperature, the c and f -like features in the correlation functions above this temperature are decoupled. We therefore interpret this temperature as the analogue of the coherence temperature in heavy-Fermion metals. At the high-temperature crossover both, the dispersionless f -like Kondo-resonance in the single-particle spectrum and the f -like low-energy spin excitation disappear. The only remaining f -like feature in the single particle spectrum are the high-energy ‘Hubbard bands’, corresponding to the ‘undressed’ transitions $f^1 \rightarrow f^0$ and $f^1 \rightarrow f^2$. We therefore interpret this second temperature as the Kondo temperature of the system.

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- [1] G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).
 - [2] P. Fulde, J. Keller, and G. Zwicknagl, Solid State Phys. **41**, 1 (1988).
 - [3] G. Aeppli and Z. Fisk, Comments Condens. Matter Phys., **16** 155 (1992).
 - [4] Z. Schlesinger *et al.*, Phys. Rev. Lett. **71**, 1748 (1993).
 - [5] M. Vekic *et al.*, Phys. Rev. Lett. **74**, 2367 (1994).
 - [6] N. Shibata *et al.*, cond-mat/9712315.
 - [7] L. Taillefer *et al.*, J. Magn. Magn. Mater. **63& 64** 372 (1987).
 - [8] J. Cooley *et al.*, Phys. Rev. Lett. **74**, 1629 (1995).
 - [9] K. Tsutsui *et al.*, Phys. Rev. Lett. **76**, 279 (1996).
 - [10] A. M. Tahvildar-Zadeh, M. Jarrel, and J. K. Freericks, e-print cond-mat/9710136.
 - [11] O. Gunnarson and K. Schönhammer, Phys. Rev. B. **28**, 4315 (1983).
 - [12] R. Eder, O. Stoica, and G. A. Sawatzky, Phys. Rev. B. **55**, 6109 (1997); see also cond-mat/9711248.
 - [13] H. Tsunetsugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. **69**, 809 (1997).
 - [14] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).